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Model Based Control of Solidification

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Abstract

In this paper, model based control of solidification is studied. A one-dimensional model that describes the dynamic response of the solidification rate for a pure substance is developed. The solidification of a metal column is controlled in order to solidify at a desired rate. The manipulated variable is the power to the heater at the top of the casting. A linear PI-controller is implemented and yields acceptable performance for the simulated case.

Keywords: Phase transition, solidification, numerical methods, model based control

1. Introduction

Phase transition in processes is an area of great technological importance in many fields, such as materials science, geology, energy processes, environmental sciences, food processing, and cryobiology. The characteristic feature of these processes is the presence of time evolving unknown boundaries separating the phases. Consequently, they belong to the class of moving boundary problems. The prototype of such problems is the Stefan problem, named after the early work of J. Stefan, who studied the melting of the polar ice cap around 1890.

In metal casting, two important characteristics that determine the quality of the finished material are the growth velocity and the local thermal conditions at the solidification front. Figure 1 shows an example of the morphology of the solid/liquid interface as a function of the growth velocity. At high growth velocities, the interface between the solid and liquid phase becomes dendritic. The dendritic morphology at the interface may cause heavy segregation of impurities between the dendrite arms during solidification (Kou 1996), and thus the concentration of impurities in the solidified metal may be dependent of the solidification velocity. Hence, it may be desirable to control the rate of solidification to a predefined value in order to make the solidified metal as pure as possible.

In this work, a one-dimensional numerical model for controlling the solidification rate in a pure substance is developed. Solidification modeling is reported in numerous papers and books. Since the advent of computers, many studies have been carried out in

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order to describe phenomena at meso- or microscale levels. Nevertheless, according to Zabaras (1999), little research has been carried out on solidification modeling for real time control purposes. Modeling for control purposes requires a simplified description of the complex processes, in order to achieve acceptable computation time. Yet, the model must be able to predict the behaviour of the system reasonably well. References to related previous work in the field of phase transition modeling will be given in the next section.

Control of solidification processes is reported in Zabaras (1990) and Zabaras et al. (1988). In these works, the control problem is adressed as an inverse problem, and a perfect model is assumed. No corrections are made due to model error and disturbances. The presence of model and parameter uncertainties are taken into account in Franke et al. (1996) where strategies to minimize a deviation error is calculated online, and action is taken by the furnace control system. Inverse Stefan problems are reported in several papers and books. Detailed information about this subject is found in Gol'dman (1997). Other works treating the inverse Stefan problem are Hoffmann and Sprekels (1982), Sagues (1982), and Jochum (1980).

This paper is organized as follows: First a brief overview of modeling strategies for two-phase transitions is presented. Then the case study process is described. After that, simulation and control of the solidification rate are discussed. Finally some conclusions are drawn.

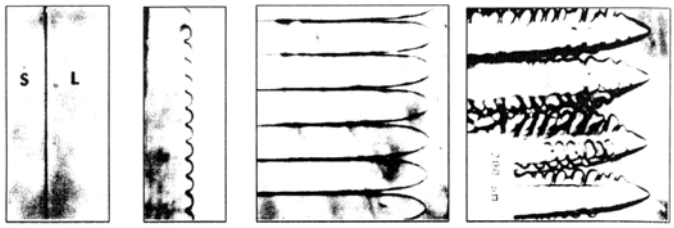

Figure 1. Example of morphology of the solid/liquid interface at different growth velocities in a transparent organic system. Taken from Stefanescu (2002).

2. Modeling strategies for two-phase transitions

Two different approaches are used in the modeling of phase transitions in a spatial domain. In the most common approach, a sharp interface between the phases is considered, defined by the phase change temperature. The total domain Ω of the substance is then divided into two separate subdomains (one for each phase), Ω_1 and Ω_2 in figure 2, and the heat and mass balance equations are formulated for each subdomain. This approach leads to one partial differential equation (PDE) for each subdomain (phase), with one boundary condition and one interface condition. The interface, or moving boundary, yields an ODE for the position of the interface.

The one-dimensional classical Stefan problem is given by (Crank 1984):

$$\frac{\partial T_i}{\partial t} = \alpha_i \frac{\partial^2 T_i}{\partial z^2} \quad \text{for } z \in \Omega_i(t), \;\; i = 1,2 \tag{1}$$

where $\alpha = k/(\rho \hat{c}_p)$ is the thermal diffusivity, T is the temperature, k is thermal conductivity, ρ is the density, and $\hat{c}_p$ is the specific heat capacity.

At the interphase between the phases, the energy balance and Fourier's law of conduction yields

$$\rho \Delta \hat{H}_f \cdot \frac{dh}{dt} = q_2\big|_{z=h} - q_1\big|_{z=h} = -k_2(\nabla T_2) + k_1(\nabla T_1), \tag{2}$$

where $\Delta \hat{H}_f$ is the latent heat, and h is the position of the interface front. The boundary condition at the interface is:

$T_1(t, z = h) = T_2(t, z = h) = T_{ch}$,

where T_{ch} is the phase-change temperature.

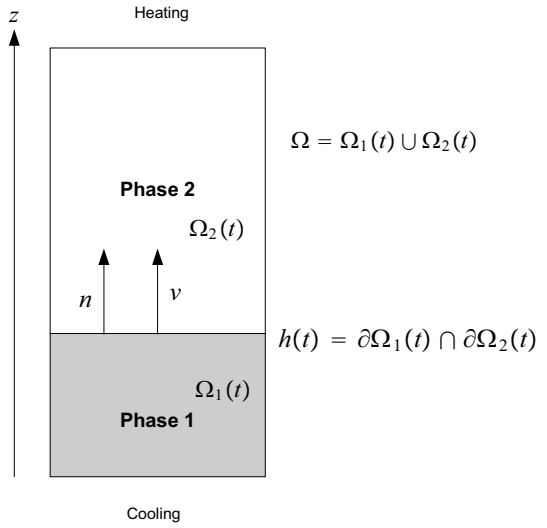

Figure 2. Simplified sketch of the two-phase transition problem. v=dh/dt is the interface velocity and n is the normal vector of the interface. In the two-domain approach, the domain is divided into two subdomains (phase 1 and 2), and the balance equations are formulated on each subdomain. In the one-domain approach, the balance equations are formulated on the whole of the domain.

Numerical methods for solution of the sharp interface approach are e.g. the level set method, fixed grid, and variable grid methods. The level set method is implemented for solidification processes in Gibou et al. (2003), whereas the method in general is described in Osher and Fedkiw (2003). Front tracking and front fixing methods are described thoroughly in Crank (1984).

In the second approach, the domain is considered as a whole, Ω in figure 2. The balance equations are then formulated on the whole of the domain; thus one PDE with

two boundary conditions are valid for the whole domain (total volume). In this approach, the phase interface position must be calculated from the solution of the PDE. Some methods mentioned in the review of Hu and Argyropoulos (1996) are the methods of latent-heat evolution, the apparent heat capacity methods, the effective capasity method, and the enthalpy method.

3. The solidification model

We consider a metal column of height L, originally in liquid form. The metal column is assumed to be fully insulated on the vertical surface. The enthalpy method is employed. In the enthalpy method, equations (1) and (2) reduce to the single equation

$$\rho \frac{\partial \hat{H}}{\partial t} = k \frac{\partial^2 T}{\partial z^2} \tag{3}$$

where H is specific enthalpy, and it is assumed that k and ρ are independent of the temperature. The temperature and enthalpy are related by the function

$$\hat{H}(T) = \begin{cases} \hat{c}_p^s (T - T_{ch}), & T \le T_{ch} \\ \hat{c}_p^l (T - T_{ch}) + \Delta \hat{H}_f & T > T_{ch} \end{cases}, \tag{4}$$

and the temperature is found from the enthalpy found by inverting equation enthalpysemperature. The model is discretized in space (fixed and uniform grid) by the method of lines, yielding a system of ODEs. The discretized system is implemented in MATLAB (2004).

A drawback of the enthalpy method is that the temperature and phase boundary dynamics become oscillatory, especially for isothermal phase changes. This is because the phase front is represented by a control volume rather than a surface (Chun and Park 2000). Works employing the enthalpy methods are found in Voller and Cross (1981) and Voller et al. (1990). In these works, the front position is located by introducing a variable called local solid fraction, which locates the discretizing element containing the front position. Voller and Cross (1983) assumed that the fraction of solid may be linearly interpolated during latent heat release for the discretizing element containing the phase front. The amplitude of the oscillations in the phase front was reduced, but the fluctuations in the temperature were not influenced. Tacke (1985) suggested an improved discretization of the enthalpy method to obtain an oscillation-free solution. In that method, however, equal material properties for both phases are assumed. In this work, the method of is extended to be valid for materials having different material properties in the two phases. This is done by using the mixture theory (Stefanescu 2002) for the grid cell containing the phase front

$$k = f_s k_s + (1 - f_s) k_\ell,$$

where k is the conductivity, f_s is the value of the improved estimate of the fraction of solid calculated by Tacke's method. The online estimate of the position is

$$h(t) = (i-1)\Delta z + f_s \Delta z, \tag{5}$$

where i is the index of the grid cell containing the phase front, and Δz is the grid size.

4. Simulation and control of the solidification rate

We now write the model as

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x},\mathbf{u}) \text{ and } \hat{y} = g(\mathbf{x},\mathbf{u}),$$

where the states are the enthalpies in the grid cells

$$\mathbf{x} = \begin{pmatrix} \hat{H}_1 & \cdots & \hat{H}_N \end{pmatrix}^T = \begin{pmatrix} x_1 & \cdots & x_N \end{pmatrix}^T$$

and $\hat{y} = g(\mathbf{x},\mathbf{u}) = h(t)$ is the estimate in equation (5).

The manipulated value is heating at the top of the casting (assuming constant cooling conditions):

$$\mathbf{u} = Q_L = u_1.$$

If we want to control the velocity, the position must track a ramp. In continuous processes, an integrator is included in the controller to achieve zero error at steady state. Even though the solidification process is a batch-process, and hence never reaches steady state, it may be advantageous to include an integrator in order to decrease the controller deviation as the time elapses.

The linear PI controller is given by

$$u_1 = K_P e + K_I \sigma,$$

where $e = s_{ref} - \hat{y}$, $s_{ref}(t) = v_{ref} \cdot t$ and $\sigma = \int e dt$. The result of the closed loop simulation is shown in figure 3. From the figure, the system appears to track the reference well.

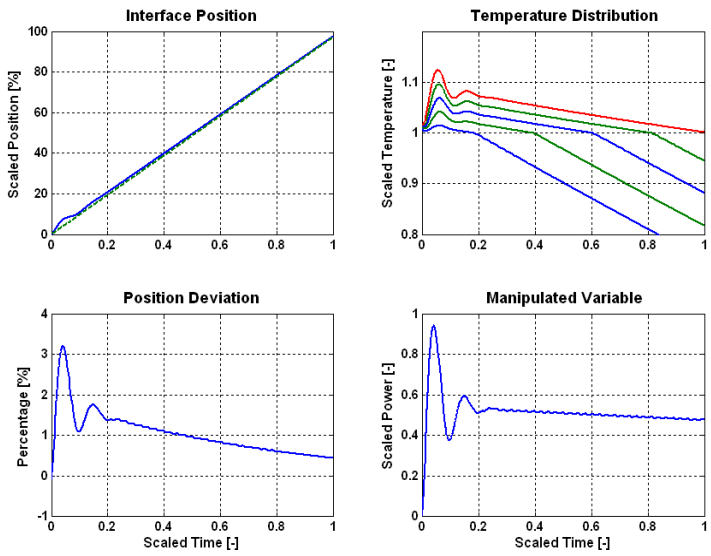

Figure 3. Control of the solidification rate for a constant reference.

5. Conclusions

The intention of this paper is to develop a fast and simple mechanistic model for the position of the solidification interface. The model is simplified to make it suitable for control purposes, and is used to develop a linear PI-controller in order to control the solidification velocity.

For the cases simulated above, the position tracks the reference well. It may be possible to extend the model and control strategy to a gas-liquid transition.

Further research will include validation with experimental plant data and comparison with other modeling methods (e.g. the level set method).

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